



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 23 30 31 32 33 34 35 36 37 38 57 58

ring nodes :

1 2 3 4 5 6 39 40 41 42 43 44 45 46 47 48 49

chain bonds :

2-7 4-30 6-57 7-58 8-9 10-11 11-12 13-14 14-15 14-16 17-18 19-20 19-21 21-23 31-32 32-33 34-35 36-37 37-38

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-43 40-41 41-42 42-43 44-45 44-49 45-46 46-47 47-48 48-49

exact/norm bonds :

2-7 4-30 6-57 7-58 8-9 10-11 11-12 13-14 14-15 14-16 17-18 19-20 19-21 21-23 31-32 32-33 34-35 36-37 37-38 39-40 39-43 40-41 41-42 42-43 44-45 44-49 45-46 46-47 47-48 48-49

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:H,Cy,Ak

G2:[*1],[*2],[*3],[*4],[*5]

G3:O,S,N

G4:[*6],[*7],[*8],[*9],[*10]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS
12:CLASS13:CLASS14:CLASS15:CLASS16:CLASS17:CLASS18:CLASS19:CLASS20:CLASS21:CLASS
23:CLASS30:CLASS31:CLASS32:CLASS33:Atom 34:CLASS35:Atom 36:CLASS37:CLASS38:CLASS
39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom
57:CLASS58:CLASS

Generic attributes :

58:

Saturation : Unsaturated